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Analysis of QSAR Models Quality

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The investigation of the quantitative structure activity/property relationships (QSAR/QSPR) of organic compounds is an essential aspect of present experimental chemistry, biochemistry, medicinal chemistry, and especiallyin drug discovery. The obtained information is composed of mathematical equations relating the chemical structure of the compounds to a wide variety of their physical, chemical and biological properties. In our previous work, QSAR study of set of various substituted hydrazones was performed to estimate the quantitative effects of the selected physicochemical descriptors on experimentally determined dissociation constant. Several statistical parameters: correlation coefficients (R^2), adjusted coefficient of correlation ($R^2_{adj.}$), mean squared error (MSE), root mean square error (RMSE) and Fischer test (F-test) were used to test the quality of the developed QSAR models. All QSAR model were statistically significant: $R^2R^2_{adj}$> 0.8, MSE < 0.003, RMSE < 0.05.Advantage of this method is when a correlation between structure and activity/property is found, any number of structurally similar compounds (compounds with hydrazine moiety), can readily be screened *in silico* for selection of structures with desired properties. As a continuation of our previous work, we tested QSAR model using different type of hydrazine compound. We calculated their pK values constant, using our models and those values were compared with their literature values.The results showed that the application of models would largely depend on the structural similarities/differences of the tested compounds compared to the compounds on which the models were constructed.

Keywords: QSAR/QSPR, hydrazones, p*K* constant, descriptors